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BsnMod: A Windows™ program for simulating basin-scale fluid flow and heat transfer processes related to sediment compaction and tectonic uplifting in two dimensions[1]

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Abstract: Sediment compaction and tectonic uplift are common driving forces for basinal fluid flow. Fluid-flow and heat-transfer processes are described by medium-continuity, fluid-continuity, and heat-conservation equations. Numerical solution of these equations simulates the evolution of porosity, permeability, fluid overpressure, flow rate, and temperature. A finite difference method, using an approximate curvilinear co-ordinate system, was described and used by previous workers with a modified numerical scheme. The same numerical scheme is used in BsnMod, but Visual C++™ is used instead of FORTRAN as the programming language. The program has a user interface allowing input on model selection (compaction, gravity), basin and grid configuration, medium properties, and boundary conditions. The output can be both graphics and spreadsheets. The graphic output consists of the grid, fluid-flow vectors, isotherms, and isobars, and can be copied to and edited by other graphic programs.

Résumé : La compaction des sédiments et le soulèvement tectonique sont des mécanismes usuels pour l'écoulement des fluides dans les bassins. L'écoulement des fluides et le transfert de chaleur sont décrits au moyen d'équations de la continuité du milieu, de la continuité du fluide et de la conservation de la chaleur. La solution numérique de ces équations donne une simulation de l'évolution de la porosité, de la perméabilité, de la surpression hydraulique, du taux d'écoulement et de la température. Une méthode des différences finies utilisant un système de coordonnées curvilinéaires approximatives a été décrite et utilisée par d'autres chercheurs avec un schéma numérique modifié. Le même schéma numérique est utilisé dans BsnMod, bien que le langage de programmation soit C++ plutôt que FORTRAN. L'interface-utilisateur du programme permet d'intervenir dans le choix des modèles (compaction, gravité), la configuration du bassin et du quadrillage, de même que le choix des propriétés du milieu et des conditions aux limites. Les données de sortie peuvent avoir la forme de documents graphiques ou de chiffrier. Les documents graphiques comprennent le quadrillage, les vecteurs d'écoulement, les isothermes et les isobars; ils peuvent être copiés et révisés par d'autres programmes graphiques.

[1] Contribution to the Appalachian Foreland and St. Lawrence Platform NATMAP Project

INTRODUCTION

Underground fluid flow and heat transfer are responsible for a variety of geological processes in sedimentary basins such as diagenesis, hydrocarbon migration, and metallic mineralization. There are essentially two methods of characterizing basinal fluid flow and heat transfer. One is to use geological and geochemical data, such as recorded by diagenetic minerals, to reconstruct the patterns and history of basinal fluid flow. The other is to use numerical methods to solve partial differential equations describing the fluid-flow and heat-transfer processes, thus quantitatively characterizing the fluid-flow systems. A common practice is to use the first method to construct conception models, and use the second method to constrain or test these models.

Among the numerous possible forces that could drive underground fluid flow in sedimentary basins, sediment compaction and topographic relief (gravity) are most important. Sediment compaction expels pore fluids out of sediments through collapse of pore space. It plays a major role in driving underground fluid flow during the early history of sedimentary basins, i.e. during the processes of sedimentation and burial. Topographic relief, however, plays a more important role in the late-stage history of a basin, mainly related to tectonic uplift.

This paper describes a computer program for solving the governing equations of sediment compaction, fluid flow, and heat transfer related to compaction-driven fluid flow. The same program also solves governing equations of fluid flow and heat transfer related to topography-driven (or gravity-driven) fluid flow. A finite difference method, using an approximate curvilinear co-ordinate system, was described by Bethke (1985) and used by Chi and Savard (1998) with a modified numerical scheme. The same numerical scheme is used in this program (BsnMod), but C++ instead of FORTRAN is used as the programming language. The governing equations and the numerical methods have been described in detail elsewhere (Bethke, 1985, 1986; Harrison and Summa, 1991; Chi and Savard, 1998), but they are nevertheless described below in order to provide a background for the program, although the focus of this paper is on the functionality of the program. It must be pointed out that the program is still in the process of refinement, and further development includes incorporation of other driving forces of fluid flow such as tectonic deformation.

GOVERNING EQUATIONS AND NUMERICAL PROCEDURE

The fluid-flow and heat-transfer processes during sedimentation and compaction are described by the following three equations according to the vertical, two-dimensional mathematical model of Bethke (1985) (*also* Bethke, 1986; Harrison and Summa, 1991):

For solid medium continuity (compaction):

$$\frac{\partial v_{zm}}{\partial z} = \frac{1}{(1-\phi)}\frac{\partial \phi}{\partial t} \tag{1}$$

For fluid continuity:

$$\phi\beta\frac{\partial \Phi}{\partial t} - \frac{1}{\rho}\left[\frac{\partial}{\partial x}\left(\frac{\rho k_x}{\mu}\frac{\partial \Phi}{\partial x}\right) + \frac{\partial}{\partial z}\left(\frac{\rho k_z}{\mu}\frac{\partial \Phi}{\partial z}\right)\right] = \phi\beta\rho V_{zm} - \frac{1}{(1-\phi)}\frac{\partial \phi}{\partial t} + \phi\alpha\frac{\partial T}{\partial t} \tag{2}$$

For heat conservation:

$$\left[\rho\phi C_f + \rho_r(1-\phi)C_r\right]\frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(K_x\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial z}\left(K_z\frac{\partial T}{\partial z}\right) + \frac{\partial}{\partial x}\left(\rho v_x C_f T\right) + \frac{\partial}{\partial z}\left(\rho v_z C_f T\right) = -\rho h_f\frac{\partial \phi}{\partial t} \tag{3}$$

where v_{zm} is settling velocity of the medium, z is the vertical co-ordinate (positive upward), x the horizontal co-ordinate, t is time, ϕ is porosity, Φ is fluid overpressure, which is defined by

$$\Phi = P + \rho z \tag{4}$$

P is fluid pressure, ρ is fluid density, ρ_r is solid matrix density, μ is viscosity, α is fluid thermal expansion coefficient, β is fluid compressibility coefficient, k_x and k_z are intrinsic permeabilities in the x and z directions, K_x and K_z are thermal conductivities in the x and z directions, T is temperature, v_x and v_z are fluid velocities in the x and z directions, C_f is fluid heat capacity, C_r is solid matrix heat capacity, and h_f is fluid enthalpy. Note that equations (2) and (3) are written in a Lagrangian reference frame which remains fixed with respect to the subsiding medium but moves through space. Thus, v_x and v_z are relative to the moving medium and not to a fixed datum in space. Equations (2), (3), and (4) apply equally well to fluid flow driven by topographic relief, except that v_{zm} is zero.

The governing equations are first transformed to a curvilinear co-ordinates system, where the z'-axis is vertical and the x'-axis is parallel to the sedimentary bedding. The transformed fluid flow and heat transfer equations are as follows (Bethke, 1985):

Fluid continuity:

$$Vb\phi\beta\frac{\partial \Phi}{\partial t} - \frac{1}{\rho}\left[\frac{\partial}{\partial x'}\left(\frac{\rho k_x \Delta z'}{\mu}\right)\Delta x' + \frac{\partial}{\partial z'}\left(\frac{\rho k_z \Delta x'}{\mu}\frac{\partial \Phi}{\partial z'}\right)\Delta z'\right] = Vb\phi\beta\rho V_{zm} - \frac{Vb}{(1-\phi)}\frac{\partial \phi}{\partial t} + \phi\alpha Vb\frac{\partial T}{\partial t} \tag{5}$$

Heat conservation:

$$Vb\left[\rho\phi C_f + \rho_r(1-\phi)C_r\right]\frac{\partial T}{\partial t} - \frac{\partial}{\partial x'}\left(K_x\Delta z'\frac{\partial T}{\partial x'}\right)\Delta x' + \frac{\partial}{\partial z'}\left(K_z\Delta x'\frac{\partial T}{\partial z'}\right)\Delta z' + \frac{\partial}{\partial x'}\left(\rho v_x \Delta z' C_f T\right)\Delta x' + \frac{\partial}{\partial z'}\left(\rho v_z \Delta x' C_f T\right)\Delta z' = \rho h_f Vb\frac{\partial \phi}{\partial t} \tag{6}$$

where *Vb* is the bulk volume of a control volume (block), and is approximated by $\Delta x' * \Delta z'$. The transformed equations (5) and (6) are then transformed to finite difference forms, with the basin being divided into a series of nodal blocks bounded by vertical and bedding-parallel lines, coincident with the z' and x' axes in the curvilinear co-ordinates, respectively. The finite difference equations of both equations (5) and (6) takes the following form:

$$A_n \psi_n + A_e \psi_e + A_s \psi_s + A_w \psi_w + A_c \psi_c = S \tag{7}$$

where A represents coefficients, Ψ is the variable to be solved, and S is the source term. The subscripts *w*, *e*, *s*, and *n* stands for western, eastern, southern, and northern boundary of a given block, respecively, and *c* stands for the central point of a block.

The coefficients for the fluid continuity equation are:

$$A_w = -\frac{1}{\rho_c}\left(\frac{\Delta z' \rho k_x}{\Delta x' \mu}\right)_w \tag{8}$$

$$A_e = -\frac{1}{\rho_c}\left(\frac{\Delta z' \rho k_x}{\Delta x' \mu}\right)_e \tag{9}$$

$$A_s = -\frac{1}{\rho_c}\left(\frac{\Delta x' \rho k_z}{\Delta z' \mu}\right)_s \tag{10}$$

$$A_n = -\frac{1}{\rho_c}\left(\frac{\Delta x' \rho k_z}{\Delta z' \mu}\right)_n \tag{11}$$

$$A_c = -(A_w + A_e + A_s + A_n) + \frac{\phi_c^{\theta} Vb^{\theta} \beta}{\Delta t} \tag{12}$$

$$S = \frac{\phi_c^{\theta} Vb^{\theta} \beta \Phi_c^{P}}{\Delta t} + Vb^{\theta} \phi_c^{\theta} \beta \rho_c^{\theta} V_{zm} - \frac{Vb^{\theta}}{(1-\phi_c^{\theta})} \frac{\phi_c^{\theta} - \phi_c^{P}}{\Delta t} + \phi_c^{\theta} \alpha Vb^{\theta} \frac{T_c^{\theta} - T_c^{P}}{\Delta t} \tag{13}$$

where the superscripts ρ and θ stands for previous time step and intermediate time step, respectively.

The coefficients for the heat conservation equation are:

$$A_w = -\left(\frac{\Delta z' K_x}{\Delta x'}\right)_w - \frac{(\Delta z' \rho v_x C_f)_w + \left|(\Delta z' \rho v_x C_f)_w\right|}{2} \tag{14}$$

$$A_e = -\left(\frac{\Delta z' K_x}{\Delta x'}\right)_e + \frac{(\Delta z' \rho v_x C_f)_e - \left|(\Delta z' \rho v_x C_f)_e\right|}{2} \tag{15}$$

$$A_n = -\left(\frac{\Delta z' K_z}{\Delta z'}\right)_n + \frac{(\Delta x' \rho v_z C_f)_n - \left|(\Delta x' \rho v_z C_f)_n\right|}{2} \tag{16}$$

$$A_s = -\left(\frac{\Delta x' K_z}{\Delta z'}\right)_s - \frac{(\Delta x' \rho v_z C_f)_s + \left|(\Delta x' \rho v_z C_f)_s\right|}{2} \tag{17}$$

$$A_c = -\left(\frac{\Delta z' K_x}{\Delta x'}\right)_w - \frac{(\Delta z' \rho v_x C_f)_w - \left|(\Delta z' \rho v_x C_f)_w\right|}{2} + \left(\frac{\Delta z' K_x}{\Delta x'}\right)_e + \frac{(\Delta z' \rho v_x C_f)_e + \left|(\Delta z' \rho v_x C_f)_e\right|}{2} + \left(\frac{\Delta x' K_z}{\Delta z'}\right)_n + \frac{(\Delta x' \rho v_z C_f)_n + \left|(\Delta x' \rho v_z C_f)_n\right|}{2} + \left(\frac{\Delta x' K_z}{\Delta z'}\right)_s - \frac{-\left|(\Delta x' \rho v_z C_f)_s\right|}{2} + \frac{Vb^{\theta}[\rho_c^{\theta} \phi_c^{\theta} C_f + \rho_r (1-\phi_c^{\theta}) C_r]}{\Delta t} \tag{18}$$

$$S = \frac{Vb^{\theta}[\rho_c^{\theta} \phi_c^{\theta} C_f + \rho_r (1-\phi_c^{\theta}) C_r] T_c^{P}}{\Delta t} - \frac{\rho^{\theta} Vb^{\theta} hf}{(1-\phi_c^{\theta})} \frac{\phi_c^{\theta} - \phi_c^{P}}{\Delta t} \tag{19}$$

The upwind method is used in the formulation of the coefficients of the heat conservation equation.

It should be noted that the above transformations from Cartesian to curvilinear co-ordinates are approximate because when sediment thickness is not equal everywhere (as is the case for most sedimentary basins), and the z' and x' axes in the curvilinear co-ordinates system are not perpendicular to each other; however, owing to the much greater width than depth of sedimentary basins, the error introduced by this approximation was thought to be small (Bethke, 1985). A more accurate transformation, using standard co-ordinate transformation coefficients (e.g. Hoffmann and Chiang, 1993; Chi and Guha, 1995) is potentially possible, but will lose the convenience of grid division inherited in the approximate method.

The numerical procedure starts with an initial condition, and proceeds with the addition of a thin layer of sediment in each time step. For each time step, the medium continuity (compaction) equation is first solved in conjunction with the following equations describing the relationship between effective depth and porosity (Bethke, 1985):

$$\phi = \phi_0 e^{z_e b} + \phi_1 \tag{20}$$

$$z_e = z + \frac{\Phi - \Phi_w}{(\rho_{sm} - \rho_w)} \tag{21}$$

where ϕ_0 is porosity at deposition, ϕ_1 is irreducible porosity, and b is an empirical parameter, z is depth (negative downward from surface), z_e is effective depth, Φ is fluid overpressure, "sc" denotes surface conditions, ρ_w and ρ_{sm} are constant densities of water and water-saturated sediments respectively. Numerical solution of equations (1), (20), and (21) yields sediment settling velocities (V_{zm}), porosities (ϕ), and the thickness of a block (Δz), which are then used to solve the fluid-flow equation to obtain fluid overpressures. Since porosity is dependent on effective depth (equation 20), which is in turn dependent on fluid overpressure (equation 21), the medium-continuity equation has to be recalculated by using the last overpressure values. Iteration between the medium-continuity and fluid-flow equations continues until the porosity values are converged. The porosity values are then used to calculate the permeability values using the following equation:

$$\log k_x = A\phi + B \tag{22}$$

$$k_x / k_z = C \tag{23}$$

where k_x and k_z are bedding-parallel and vertical permeability, respectively, and A, B, and C are lithology-dependent constants (Bethke, 1985; Harrison and Summa, 1991; Kaufman, 1994). The numerical solution then proceeds to solve the heat-transfer equation to obtain temperature values. The alternating direction implicit (ADI) method (*see* Jaluria and Torrance, 1986) is used in the solution of both the fluid-continuity and heat-conservation equations. The ADI method gives rise to tridiagonal matrices for the two alternating directions and the computation scheme is very efficient. The properties of the fluid and solid medium are updated at the end of each time step. Because the fluid-saturated medium is composed of various lithological elements, the porosity and permeability values of a given block need to be averaged from the values of individual components. Geometric mean is used for heat conductivity and bedding-parallel permeability, whereas harmonic mean is used for vertical permeability to account for the barrier effect of low-permeability beds.

When all three equations (medium continuity, fluid continuity, and heat conservation) are solved, a new time step starts, and so on. A new layer of nodal blocks is created when a target thickness (defined by the total number of layers of blocks) is reached. When the calculation is complete (i.e. at a given time step), a finite number of blocks were created, with results of porosity, fluid overpressure, temperature, etc. being solved for the central point of each block.

STRUCTURE OF THE PROGRAM

The program was written with Microsoft Visual C++™ 5, using the MFC™ AppWizard (exe). Its framework is based on the document/view architecture, as for most Windows™ programs (Horton, 1997). The Single Document Interface (SDI) is used, which means that only one document can be opened at a time. This choice of program architecture is justified by the fact that the calculation is very time consuming, and it does not make sense to have several documents opened at the same time. Most data and calculation functions (e.g. the functions for calculating overpressure, temperature, etc.) are members of the document class.

Single Document Interface usually has only one view; however, in order to view both the input and output of the program, BsnMod has three views attached to the single document: one for input, one for graphical output, and one for spreadsheet output. The views for input and spreadsheet output are derived from CFormView, and the view for graphic output is derived from CScrollView. CMSFlexGrid is used for the spreedsheet input and output, with editing function being added by a floating text editor using CEdit. The switching of views was implemented in a function in the application class.

The arrays for holding various variables and coefficients are dynamically created according to the input from the user (mainly related to the total number of blocks). These arrays are automatically deleted in quitting the program, using the destructors of various classes.

The program is multithreaded, thus allowing the user to switch to other programs (e.g. MS Word) while the BsnMod program is running. Because the calculation is long and does not need user interference, a worker thread is used to handle the calculation. The worker thread is created using the function AfxBeginThread () (Blaszczak, 1997). The worker thread is declared a friend of the document class (which is responsible for holding most data) in order to access all the members of that class.

The storage of calculation results in a file is made possible through the implementation of the Serialize() function of the document class. The graphic outputs can be copied and pasted in other graphic programs such as CorelDraw™ for further editing. This was done by using several API functions for data transfer through the Clipboard. The graphics are transferred as enhanced metafiles (Petzold, 1996).

FUNCTIONALITY OF THE PROGRAM

The interface for inputting data contains eight control buttons (Fig. 1). Seven of them are for inputting data and one is for starting the calculation. The seven input buttons are for selection of models and for specification of basin configuration, fluid properties, solid properties, porosity and permeability, boundary conditions, and numerical parameters.

The "Model" button allows selection of one of three models, i.e. compaction model, stable-(steady-state)gravity model, and transient-gravity model. The default model is the compaction model.

When the "Basin data" button is pressed, a dialogue appears for specification of grid and basin configuration. The dialogue differs between the compaction model and the gravity models. If the compaction model has been selected, then the dialogue invoked by the "Basin data" button will ask for specification of the number of columns, the horizontal width

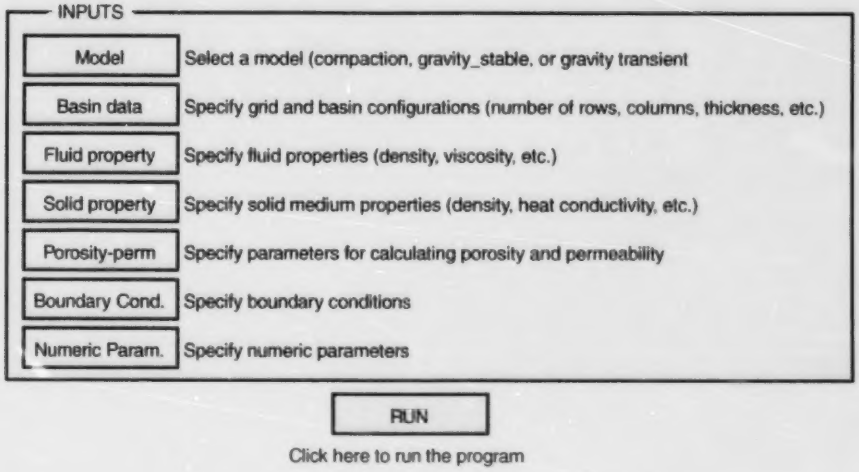

Figure 1. *The user interface of BsnMod for inputting data.*

between columns, and the total number of hydrogeological layers. When these data are entered and the "OK" button is pressed, a spreadsheet will appear, allowing input of the following data: duration of time of sedimentation, the number of time steps and the number of rows of blocks to be used in calculation, and the decompaction factor for each of the hydrogeological layers, as well as the thickness and lithological components of the hydrogeological layer at each column. The five basic lithological elements are sandstone, shale, platform limestone, reef limestone, and evaporite (Kaufman, 1994). If the stable or transient-gravity model has been selected, then the dialogue invoked by the "Basin data" button will ask for specification of the number of columns, the number of rows, the horizontal width between columns, the total number of time steps, and the duration of each time step (for stable-gravity model, the latter two data are not needed). When these data are entered and the "OK" button is pressed, a spreadsheet will appear for input of thickness, permeability, and heat-conductivity values for each block.

The data entered from the "Basin data" button are essential for determining the size of the arrays for holding data. Most of the arrays are dynamically created immediately after the specification of these data. Thus, if one skips the "Basin data" button and tries to run the program, a message will appear saying that the basin data have not been entered.

The "Fluid property" button invites inputting data related to fluid properties, including density, viscosity, thermal-expansion coefficient, compressibility coefficient, heat capacity, and heat conductivity. The "Solid property" button brings up a dialogue for entering the data related to properties of the solid medium, including density, heat capacity, and heat conductivity. Default values are shown in appropriate entries, and usually does not need modification.

The "Porosity-perm" button brings up a dialogue for entering coefficients related to porosity and permeability calculation as indicated in equations (20), (22), and (23). Although default values are shown for each of the five basic lithological components (sandstone, shale, platform limestone, reef limestone, and evaporite), it should be noted that significant variation in the values of these coefficients have been reported in the literature. In fact, the calculation results are largely dependent on the selection of these coefficients.

The "Boundary Cond." button allows specifications of the boundary conditions. The left boundary (basin centre) is considered as a symmetric plane, and no fluid flow or heat transfer occurs across this boundary. The right boundary can be either closed (no flow and heat transfer) or open (constant overpressure and temperature). The bottom boundary is closed to fluid flow and is subject to a heat flux. The heat flux can be uniformly distributed or it can vary from column to column. The upper boundary is always open to flow, and has a fixed temperature. The fluid overpressure on the surface (i.e. upper boundary) can be uniform or variable (reflecting topographic relief).

The "Numeric Param." button is for specifying the θ values (for calculating variables between two time steps) and the criteria for convergence.

The "RUN" button starts the calculation. Once this button is pressed, the user can switch to other programs to work on other things. When the computation is finished, a message will be shown to indicate the termination of the calculation. If the calculation is still going on, and one of the input buttons is pressed, a message will be shown to indicate that the calculation has not finished.

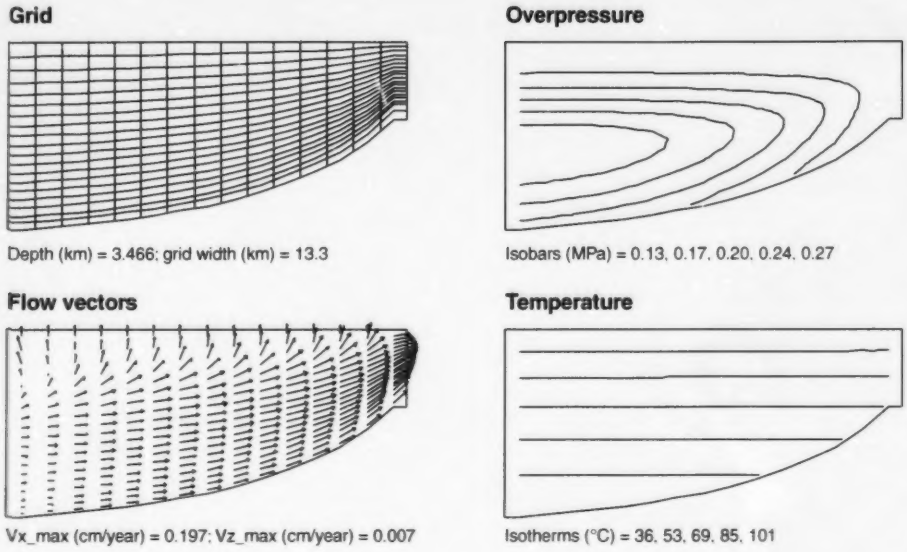
Grid
Depth (km) = 3.466; grid width (km) = 13.3
Overpressure
Isobars (MPa) = 0.13, 0.17, 0.20, 0.24, 0.27
Flow vectors
Vx_max (cm/year) = 0.197; Vz_max (cm/year) = 0.007
Temperature
Isotherms (°C) = 36, 53, 69, 85, 101

Figure 2. *An example of graphic output of BsnMod. The sediments consist of half shale and half sandstone, and were deposited over a period of 100 millions years. Fluid and solid properties as well as porosity-permeability coefficients are the same as Bethke (1985).*

Once the calculation is finished, the user can switch to one of the two output views. On the other hand, if the calculation is not finished and one of the output views is clicked, a message will indicate that no results are ready for output.

The spreadsheet output displays the results of calculation for each of the blocks. The variables to be displayed include the horizontal and vertical co-ordinates, overpressure, temperature, fluid-flow velocity, porosity, permeability, and sediment-settling velocity.

The graphic output consists of four components, i.e. the grids, flow vectors, isotherms, and isobars (example given in Fig. 2). The number of isotherms and isobars can be specified by the user. The flow vectors reflect the real direction of fluid flow relative to the medium, and the length of the vectors is proportional to the log value of the vectors. The graphic output can be copied and pasted in other graphic programs such as CorelDraw™ for editing.

SUMMARY

BsnMod is a Windows™ program for simulating basin-scale fluid-flow and heat-transfer processes in sedimentary basins. Three models that can be modelled in the present version of the program are compaction-driven, gravity-driven (stable), and gravity-driven (transient) systems. The numerical procedure is based on an approximate co-ordinates transformation and a finite difference method described by Bethke (1985) and previously used by Chi and Savard (1998). BsnMod, however, has the advantage over the previous FORTRAN program of Chi and Savard (1998) in that it has a more user-friendly interface both for input and output. The graphic output allows an immediate evaluation of the calculation results, and editing of the figures with other graphic software. Moreover, BsnMod is multithreaded, allowing the user to switch to other programs while the numerical calculation continues.

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